Glenn T. Seaborg Center Seminar

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A Simple Approach to Dynamics of Molecules with Strong Electron Correlations

Wednesday, April 28, 2004
4 pm
Building 70A-3377

Abstract

In this talk, I will describe efforts of my group to develop a simple approach for the studies of dynamics of molecules with strong electron correlations deriving from transition metal (or lanthanide/actinide ions). The approach is to map to an Anderson impurity Hamiltonian model for the molecule, treating strong correlations on the metal site well, while neglecting those on the ligands. Model parameters are derived from first principles calculations using, e.g., density functional theory. Wave functions and spectra can be computed from well established methods for this ubiquitous many body model. This approach has been used with great success for modeling spectra in rare earth intermetallics and transition metal oxides over the last two decades by, e.g., Gunnarsson and Schoenhammer, and Zaanen and Sawatsky. I will report on applications of the method to go after spectra and energetics for a cobalt based valence tautomer molecule, and for Born-Oppenheimer surfaces of the $Co^{+2}(NH_3)_6$- $Co^{+3}(NH_3)_6$ electron transfer reaction, as well as a progress report on our efforts to develop a fully atoms-to-spectra implementation of the program for absorption spectra of correlated molecules, which goes beyond the successful existing t-t multiplets program of deGroot in the realistic treatment of ligand states.

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